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QUASI-BINARY DECISION MAKING USING LIGHT SCATTERING

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RECENT PUBLICATIONS, SUBMITTAL FOR PUBLICATION AND PRESENTATIONS:

[1] P. Hu, M. Lax, "Single Scattering Inversion Problem", in Proceedings of the 1990 CRDEC Scientific Conference on Obscuration and Aerosol Research.

[2] B. Yudanin, M. Lax, "POST Adaptation for a Numerical Solution of the Spherically-Symmetric Riemann Problem," J. Mod. Phys. 285-298 (1990).

[3] B. Yudanin, P. Hu, M. Lax, "Numerical Solution of the Riemann Problem in the Presence of an External Energy Source", in Proceedings of the 1988 CRDEC Scientific Conference on Obscuration and Aerosol Research.

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[5] B. Yudanin, M. Lax, "Hydrodynamical Response to Uniform Laser Absorption in a Droplet," in Proceedings of the CRDC 1985 Scientific Conference on Obscuration and Aerosol Research, edited by R. H. Kohl and D. Stroud (1985).

Abstract

Inversion of light scattering by a single spherical scatterer with or without a layered structure is studied. By numerical simulation of the statistical properties of experiments, we can select those angles that will maximize the ability of the experiment to resolve a sphere from a layered scatterer. Applying statistical decision theory, we obtain a criterion for decision making that minimizes the probability of incorrect guesses.

Introduction

Inversion problems have existed in various branches of engineering and physics for a long time, but in the past twenty years they have received far more attention than ever before because of the available of high speed computers. In the present paper, we are going to invert light scattering information to recognize an inner structure of a spherical object. Because intensities of scattering light are highly nonlinear functions of the size and index of the scatterer, and noise is present, arbitrary pattern recognization is difficult. We will restrict ourselves to distinguishing two kinds of refraction index patterns (uniform or a layered sphere) with a range of parameters. We assume that the scatterer may be one of two kinds of objects: a sphere with a uniform refractive index or a layered sphere with different refraction indices for the core and shell, respectively. Our problems are: (1) For given experimental conditions, is there enough information to make a decision? What is the best choice of angles to yield the most significant statistics. (2) For given experimental data, how should one make a decision that minimizes wrong guesses.

We assume that we already know the following facts: The wave length λ of the light in vacuum is .4416 microns. For the u= uniform sphere (hypotheses 1), the varying parameters are the radius R^u and refraction index n^u, in the ranges $4 \leq R^u/\lambda \leq 8$ and $1.33 \leq n^u \leq 1.8$. For the l= layered sphere (hypotheses 2), the varying parameters are the inner radius R^l_{in}, core and shell refraction indices n^l_{in} and n^l_{out}. They are in the ranges $4 \leq R^l_{in}/\lambda \leq 7$, $1.33 \leq n^l_{in} \leq 1.5$ and $1.55 \leq n^l_{out} \leq 1.8$. The outer radius R^l_{out} of the layered sphere is fixed at $R^l_{out}/\lambda = 8$. Moreover, we assume there is a Gaussian noise added to the scattered intensity with $\sigma/I = 0.1$, where σ is the width of the intensity distribution of the Gaussian noise and I is the mean intensity of the light scattered at a given angle.

The method of examining general experimental data to decide between two hypotheses is a classic problem in decision theory. A procedure in the absence of a priori information was proposed by Neyman and Pearson[1] in 1933. Their results are expressed in terms of "maximum likelihood ratios". An excellent overview is given by Kendall and Stuart[2]. A readable description of the Bayes theorem approach to the same problem is given by van Trees[3]. The close connection between these two approaches is touched on by Middleton[4] in his section on binary detection systems.

Our problem is more general, in that we must estimate some continuous parameters first, in order to make the best binary decision. In the present application, these parameters are radii and indices of refraction. Thus our problem mixes continuous parameter estimation with discrete parameter detection.

Distinguishability

We propose to study the statistical properties so that we may obtain a criterion for measuring the distinguishability.

Suppose the experimental light scattering data have been taken at (spherical) scattering angles θ_i and $\phi=0$; the intensity of the scattering light per unit solid angle is denoted as $I(\theta_i)$. We want to relate the observation information to the structure of the scatterer. Because noise is always involved and can not be separated from the experimental data, it will mix the two hypotheses such that they can not be distinguished when the noise level is relatively high. The noise level depends on the experimental apparatus, the environment and the kind of data taken. For a given apparatus and environment, we should measure such data to minimize the relative noise level.

For a single scattering process, the data measured at different angles are not independent; they are correlated through complex formulas (Mie scattering for a sphere and shell). Because of the complex relationships of the scattering formulas, we can not analytically solve and will use numerical simulations to our problem.

Let's say the object is a uniform sphere with the parameter element $\eta^{(1)} \in \{R^u, n^u\}$ in the allowed range and the experimental observation is taken at M angles $\theta_1, \ldots, \theta_M$. Here M is a moderate number of order 10. We can regard the scattering as a mapping from the parameter space $\eta^{(1)}$ to an M dimensional observation space $L^M=\{I(\theta_1),\ldots,I(\theta_M)\}$. Because noise is present, one point in η space maps to an M dimensional "box" in L^M space. A similar mapping also applies for a layered object. If, at each angle θ_i, separate measurements with P different polarization intensities are made, corresponding to different polarization of the incident and scattered beam, then PM will be the dimension for the observation space. For simplicity of notation, however, we do not always introduce an explicit polarization index.

In the following, we will define a resolution criterion. First, we generate a set $\{\eta^{(j)}\}$ which includes N elements of random parameters $\eta_m^{(j)}$ in the allowed ranges for hypothesis j (j=1 for uniform sphere and j=2 for layered object), where m=1,...N. Here N is a large number of order 1000. The mth element $\eta_m^{(1)}$ of the uniform sphere set $\{\eta^{(1)}\}$ has two parameters R^u and n_m^u, and the mth element $\eta_m^{(2)}$ of the layered object set $\{\eta^{(2)}\}$ contains three parameters $R_{m,\mathrm{in}}^l$, $n_{m,\mathrm{in}}^l$ and $n_{m,\mathrm{out}}^l$. With the added noise, one image for each of the two sets $\{\eta^{(1)}\}$ and $\{\eta^{(2)}\}$ are obtained in the observation space L^M. Within the overlap region of the two images in the observation space L^M the two kinds of objects are indistinguishable from the given M intensity measurements. We will give the definition of overlap later. An event producing an image in the overlap region of the observation space is regarded as an indistinguishable event for the two hypotheses. Counting the number of the events which overlap in the observation space, we may get a measure of indistinguishability between the two cases. The ratio of the number of overlapped events to the total number events represents a measure of the indistinguishability.

We study the probability properties of the two hypotheses. In the observation space, an image point from one hypothesis can always have a probability of overlap with the an image of the other kind of hypothesis. Therefore we need to precisely define overlap of images in the observation space. We use $N(I(\theta))$ for the number of events such the intensity is in the range of $I(\theta)$ to $I(\theta)+dI(\theta)$ and N for the total number of events. We then define an overlap function:

$$F_p(\theta, I_p; \{\eta^{(1)}\}, \{\eta^{(2)}\}) = \left[\frac{\tilde{N}(I_p^{(1)}(\theta, \{\eta^{(1)}\}))}{N} \frac{\tilde{N}(I_p^{(2)}(\theta, \{\eta^{(2)}\}))}{N} \right]^{1/2} \tag{1}$$

where the subscript p denotes the polarization and the superscript (1) and (2) are for different hypotheses. The set of N (~1000) points in $\{\eta^{(j)}\}$ possesses a subset $[\eta^{(j)}(\theta_i)]$ which overlap in the sense that it may no longer be possible to distinguish whether case $j=1$ or $j=2$ is the correct with respect to a single measurement. We can choose a threshold $\alpha_{i,p}$ of indistinguishability for θ_i and measured intensity I_p by using the criteria

$$F(\theta_i, I_p; \{\eta^{(1)}\}, \{\eta^{(2)}\}) \geq \alpha_{i,p} \quad \text{for all} \quad \eta_m^{(j)} \in \{\eta^{(j)}\} \tag{2}$$

to determine the elements of subset $[\eta^{(j)}(\theta_i)]$. For observations at many angles, the joint set of subsets for all measured angles

$$[\eta^{(1)}(\theta_1, \ldots, \theta_n)] = \bigcap_{i=1}^{n} [\eta^{(1)}(\theta_i)] \tag{3}$$

measures the overall fuzziness of the experiment. As an application, we assume the measurement is taken at given angles θ=25, 40, 90, 105, 125, 140 for two polarizations (12 measurements). For simplicity we set all $\alpha_{i,p}$ to be the same $\alpha_{i,p}=\alpha$. In Fig. 1 we show the original set (dots) of parameters for the uniform sphere chosen by Monte Carlo techniques, and its joint subset for 12 measurements (triangles). The ratio of the numbers of the elements of the joint subset and the original set is about 10%. Therefore, about 90% of uniform sphere events (the dots not covered by the triangle in Fig. 1) are distinguishable from the layered events in the L^{12} space. The superscript 12 is the number of dimensions of the observation space, that is the number of measurements. The remaining 10% of the events for the uniform sphere (the triangles in Fig. 1) are indistinguishable from the layered scatterer for the given set of 12 measurements.

To produces a better resolution between these two hypotheses, a trivial approach is to increase the number of the detectors so that the events in the new space L^M (M>12) will not overlap as much as in the original space L^{12}. In most experiments, distinguishability is limited by the number of detectors. To make the most of the equipment for a better resolution, one can rearrange the detectors for some optimized angles so that the number of the elements in the joint subset is minimized. This can be done by the following iteration procedure: First we randomly generate two parameter sets $\{\eta^{(1)}\}$ and $\{\eta^{(2)}\}$ as initial sampling sets. Use Eq. (4) below to find the best angle θ_1 by taking a minimum of the overlap function F for two polarizations over θ_1. Substitute θ_1 and the original sampling sets into Eq. (5), below, to obtain the subsets $[\eta^{(1)}(\theta_1)]$ and $[\eta^{(2)}(\theta_1)]$ by Eq. (5). Iterating this procedure by using the new sets $[\eta^{(i)}(\theta_1)]$ in Eqs. (4)

and (5), we will obtain the second best angle θ_2 and the subset $[\eta^{(j)}(\theta_1,\theta_2)]$. Repeat the iteration procedure (4) and (5) for angles $\theta_1, \theta_2, \theta_3, \cdots$ until the number of elements of the joint subset $[\eta^{(i)}(\theta_1,.....,\theta_n)]$ is less than a desired value. With the optimization completed for i-1 angles, we can optimaize over θ_i using:

$$\min_{\theta_i} \prod_{p=1}^{2} \int_0^{\infty} dI\, F_p(\theta_i, I_p; [\eta^{(1)}(\theta_1,.....,\theta_{i-1})], [\eta^{(2)}(\theta_1,.....,\theta_{i-1})]) \tag{4}$$

$$\eta_m^{(j)} \in [\eta^{(j)}(\theta_1,.....,\theta_{i-1},\theta_i)] \quad \text{if} \quad F_p(\theta_i, I_p; [\eta^{(1)}(\theta_1,.....,\theta_{i-1})], [\eta^{(2)}(\theta_1,.....,\theta_{i-1})]) \geq \alpha_{i,p}$$

$$\text{for all} \quad \eta_m^{(j)} \in [\eta^{(j)}(\theta_1,.....,\theta_{i-1})] \tag{5}$$

Here we assumed that intensities of two polarizations (the subscript p) for each angle have been measured.

Decision

In this section, we apply statistical decision theory to the inversion problem. Let H_1 and H_2 denote the two hypotheses; 1 for the uniform sphere and 2 for the layered sphere. Suppose we have obtained a set of experimental data for the intensities at several angles $I_{\exp}(\theta_i)$. We want to decide which class (uniform sphere or layered object) the scatterer belongs to. We can use the least square fit to find the best fit for the hypothesis h:

$$v_h = \min_{\eta^{(h)}} \sum_i \left\{ I_{\exp}(\theta_i) - I(\theta_i, \eta^{(h)}) \right\}^2 \tag{6}$$

within the permitted parameter space. A simple statistic to decide between these cases can be chosen as $v_1 - v_2$. Suppose the experimental data are from a uniform sphere, k=1. Then v_1 is dominated by the experimental noise, usually a small value, while v_2 is a large value because it is not dominated by noise but by the shift because of an incorrectly chosen hypothesis. For some experimental data the fitting with wrong hypothesis may be small if the number of the detectors is not large enough. The wrong fitting value of v covers a large range of a uniform scale space. Therefore we use a log scale for the statistic

$$R = \log_{10}(v_1/v_2)$$

to decide between the two hypotheses. The decision rule can be obtained as follows. Let's assume we know the the conditional probability $P(R \mid H_h)$ of getting R under hypothesis h. According to Neyman-Pearson[1-4], when a priori probability and the cost of the decision are unknown, we may use a constraint condition on the probability P_F, of a "false alarm" is:

$$P_F = \alpha = \int_{\lambda}^{\infty} P(R \mid H_1)\, dR \tag{7}$$

to find the threshold λ, where α is the value permitted for a false alarm (we say H_2 while H_1 is true). After finding the threshold, we shall make decision by the criterion:

$$\text{if } \Lambda(R)>\lambda \quad \text{choose } H_2 \tag{8}$$

$$\text{if } \Lambda(R)<\lambda \quad \text{choose } H_1 \tag{9}$$

where

$$\Lambda(R)=P(R \mid H_1)/P(R \mid H_2) \tag{10}$$

is the maximum likelihood ratio.

The conditional probabilities, $P(R \mid H_h)$, can be obtained (ahead of time) by numerical simulation. As an application, we generate a set consisting of 1000 elements of random parameters for each hypothesis. We then calculate the intensities of the light scattering for these parameters at the angles θ=90, 105, ,120, 135, 150, 165 for both parallel and perpendicular polarizations. Finally we add 10% noise to the calculated intensities and regard the result as pseudo experimental data. To get the distribution profiles for both cases, we also use the least square method

$$v_h^s = \min_{\eta^{(h)}} \sum_i \left[I_{\exp}^s(\theta_i) - I(\theta_i, \eta^{(h)}) \right]^2 \tag{11}$$

to fit the pseudo experimental data with the best parameter $\eta^{(h)}$. Here $I_{\exp}^s$ was computed for source s (pseudo experimental data). v_h^s is the best least square fit for a set of experimental data of source s by the hypothesis h within the permitted paramete... Because we used wide ranges for the parameters, the intensities have hundreds of oscillations over the varying parameters. It is difficult to locate a global minimum for v_h^s, because it has hundreds of oscillations over the varying parameters. To make the programs more efficient, we made lookup tables for the Bessel and Legendre functions. Defining $R^s=\log_{10}(v_1^s/v_2^s)$ and counting the number of the events in which R^s falls into the interval $(R,R+dR)$, denoted as $\tilde{N}(R^s)$, we obtain the distribution profile for the source s. In Fig. 2, $N(R^s)$ vs R^s is plotted for both sources. The left profile of this figure is for the source s=1 the uniform sphere, while the right one is for the source s=2 the layered object. The small overlap between the two curves in Fig. 2. shows that the resolution of these two cases is quite good.

[1] J. Neyman and E. S. Pearson, "On the Problem of the Most Efficient Tests of Statistical Hypotheses," Philosophical Trans. A, 231, 289 (1933)

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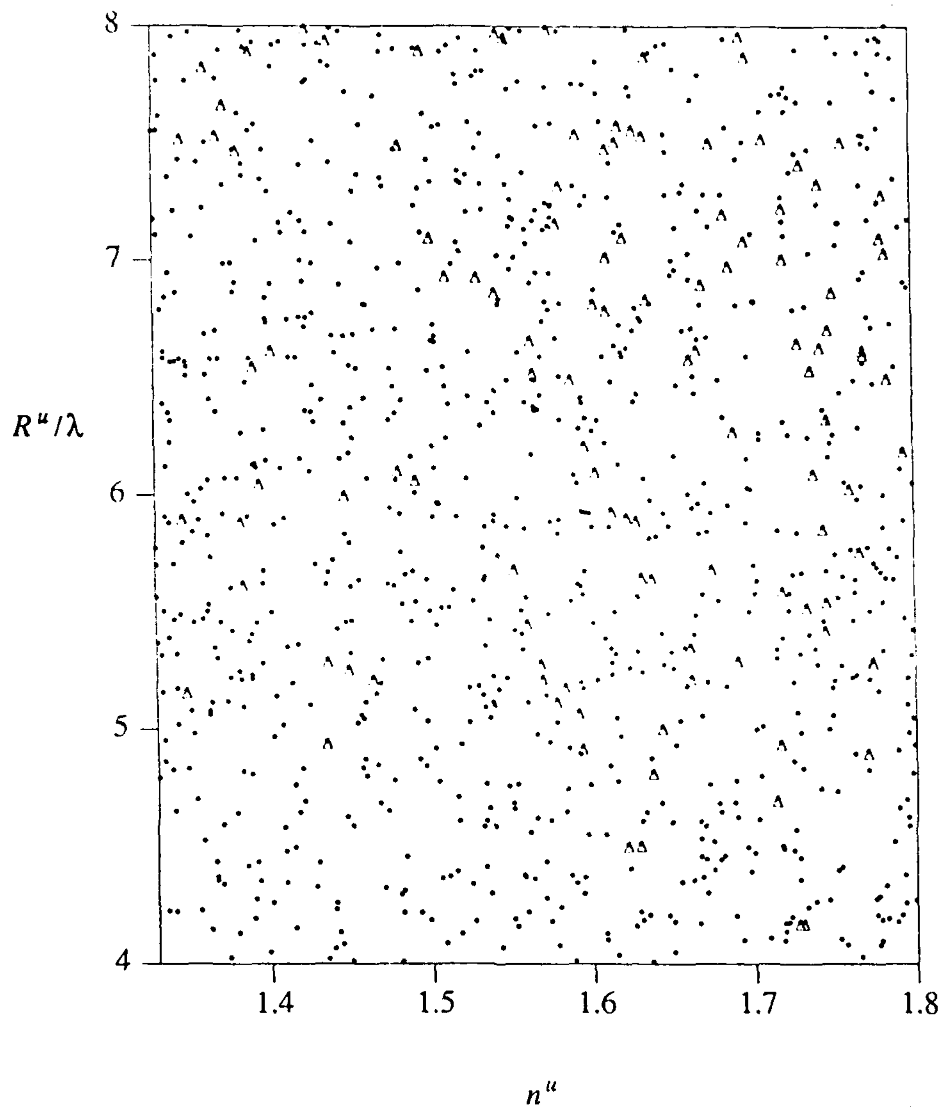

Fig. 1. Joint subset and original parameter set for the uniform sphere. The vertical scale is for R^u/λ. The 1000 dots (and triangles) are randomly selected from the available parameter set $\{\eta^{(1)}\}$ for the uniform sphere. The triangles are for the elements of the joint subset of uniform sphere for the 6 given angles and two polarizations; they are the points indistinguishable from the layered objects. The ratio of the numbers of the triangles and dots is about 10%, or about 90% of the uniform sphere events are distinguishable from layered objects. The original parameter set consists 1000 elements, each one has two components of random numbers for the parameters of the uniform sphere. The two parameters are the radius and refraction index in the ranges of $4 \le R^u/\lambda <= 8$ and $1.33 \le n^u \le 1.8$. The measurements are taken for the intensities of two polarizations (parallel and perpendicular) at 6 angles θ=25, 40, 90, 105, 125, 140.

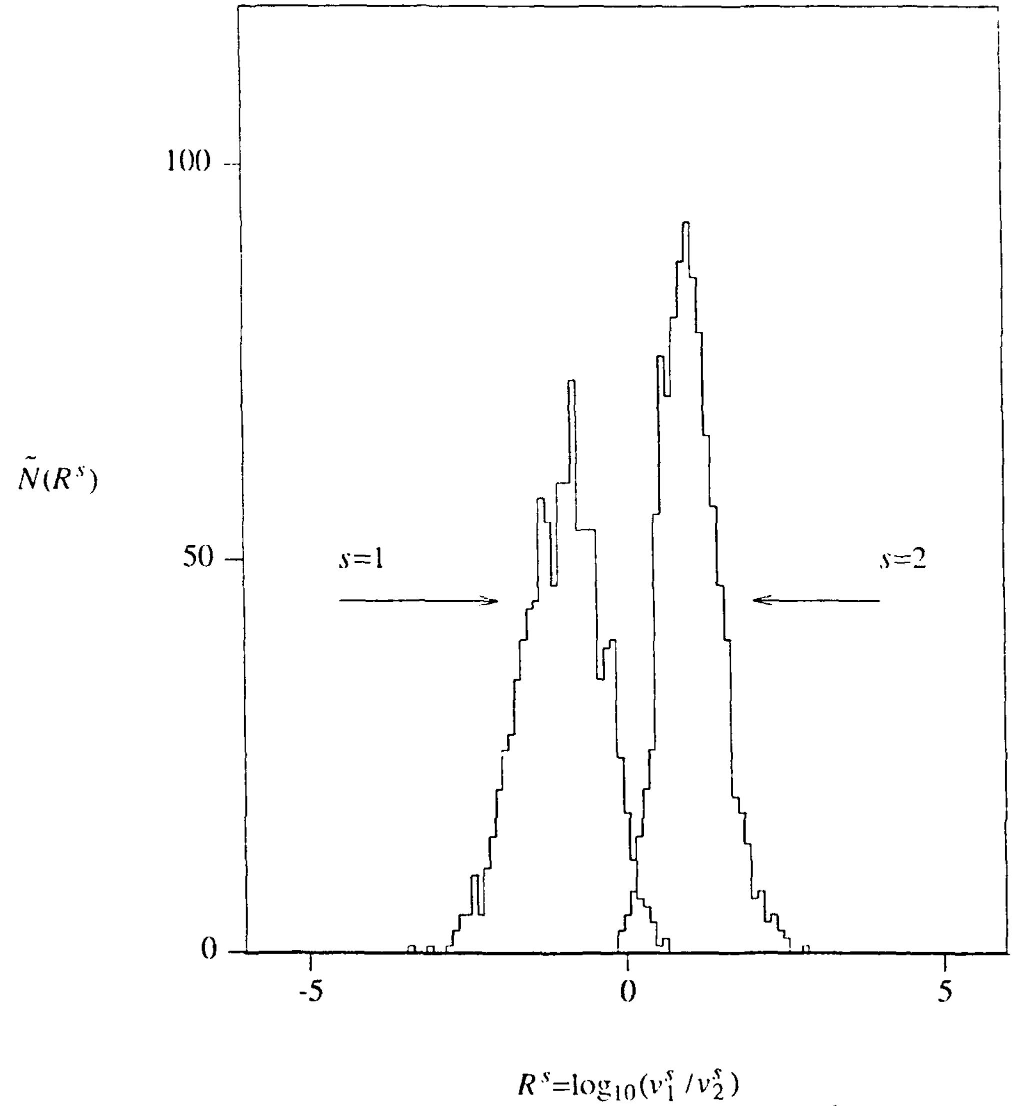

Fig. 2. Distribution profiles. The vertical axis is $\tilde{N}(R^s)$ the number of events per unit R, $dR=0.1$ is used. The left profile is the distribution profile for the appropriate for uniform spherical source, while the right one is for the layered scatterer. The measurements are taken for the intensities of two polarizations (parallel and perpendicular) at 6 angles θ=90, 105, 120, 135, 150, 165 with 10% noise. The uncertainty of the parameter ranges are follows: For the sphere, the two parameters are the radius and refraction index in the ranges of $4 \leq R^u/\lambda \leq 8$ and $1.33 \leq n^u \leq 1.8$. For the layered object, the three parameters are the inner radius and refraction indices in the ranges of $4 \leq R^l_{in}/\lambda \leq 7$, $1.33 \leq n^l_{in} \leq 1.5$ and $1.55 \leq n^l_{in} \leq 1.8$.